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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Group Art Unit: 2193
 Examiner: Michael Yarry
 Application No.: 10/524,191
 Filing Date: June 5, 2006
 Applicant: Christian BARTELS
 Title: INCREMENTAL UMBRELLA SAMPLING,(AS AMENDMED)
 Attorney Docket: 37960-000107/US

Via facsimile to: 001-571-273-8300
 Commissioner for Patents
 Randolph Building
 401 Dulany Street
 Alexandria, VA 22314
 U.S.A.

Date: October 17, 2010

Response after final

Dear Mr. Yarry,

In response to the final Office Action mailed on September 13, 2010, the following remarks are respectfully submitted in connection with the above-identified application.

The applicant wishes to thank the Examiner for the telephone interview. During the interview the applicant summarized the claims and explained differences between the claims filed by the applicants representative with the response dated July 21, 2010, and the applicants paper "Multidimensional Adaptive Umbrella Sampling: Applications to Main Chain and Side Chain Peptide Conformations".

As to the differences, the claims expose a method that relies on weighting factors (weighting factors times a function of the states) in the fitting step, whereas the paper relies on potentials of mean force. Potentials of mean force and weighting factors are fundamentally different, e.g.,

- Knowing the weighting factors, potentials of mean force can be calculated (e.g., equations 18 and 2 in the paper). In contrast, it is impossible to derive weighting factors from the potential of mean force.
- When using the weighting factors in the fitting step, the resulting iterative sampling scheme can be used to direct sampling into regions that were comparatively little sampled in previous iterations. This is not possible, when using potentials of mean force.

The Examiner confirmed that after receiving a letter from the applicant, he would reconsider the application, consult with his advisor and give a response within a short time, wherein the response would be different from the previous one. If the Examiner has further questions, he is invited to contact the applicant by e-mail at hanschristian.bartels@gmail.com.

Respectfully submitted



Christian BARTELS, Applicant